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NEWS	11	APR 02	DWPI: New display format ALLSTR available
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NEWS EXPRESS FEBRUARY 15 10 CURRENT WINDOWS VERSION IS V8.4.2,
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* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:11:05 ON 21 APR 2010

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.22	0.22

FILE 'REGISTRY' ENTERED AT 15:11:27 ON 21 APR 2010

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 APR 2010 HIGHEST RN 1219791-89-5
DICTIONARY FILE UPDATES: 20 APR 2010 HIGHEST RN 1219791-89-5

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TSCA INFORMATION NOW CURRENT THROUGH January 8, 2010.

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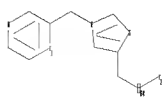
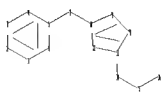
http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\STNEXP\Queries\10593910 generic.str





chain nodes :
7 14 15 16
ring nodes :

1 2 3 4 5 6 8 9 10 11 12
chain bonds :
5-7 7-8 11-14 14-15 15-16
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 7-8 8-9 8-12 9-10 10-11 11-12 11-14 14-15
15-16

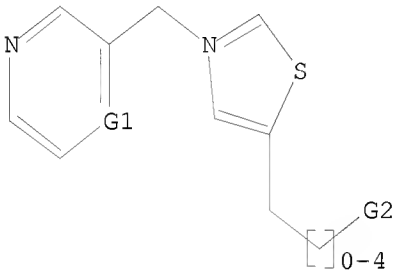
G1:C,N

G2:O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 14:CLASS 15:CLASS 16:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 C,N
G2 O,N

Structure attributes must be viewed using STN Express query preparation.

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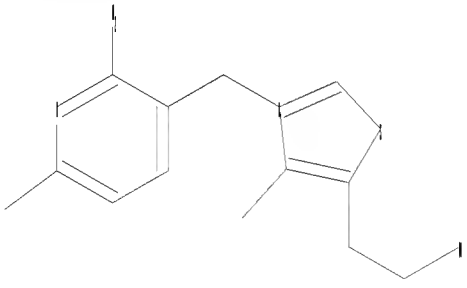
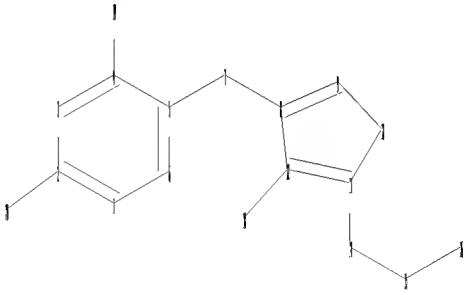
Uploading C:\Program Files\STNEXP\Queries\10593910 elected.str





chain nodes :
7 14 15 16 18 19 20
ring nodes :
1 2 3 4 5 6 8 9 10 11 12

chain bonds :
2-20 4-19 5-7 7-8 11-14 12-18 14-15 15-16
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12
exact/norm bonds :
4-19 7-8 8-9 8-12 9-10 10-11 11-12 15-16
exact bonds :
2-20 5-7 11-14 12-18 14-15
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

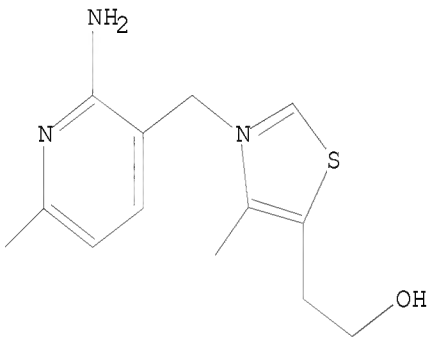
G1:C,N

G2:O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS 20:CLASS

L2 STRUCTURE UPLOADED

=> d l2
L2 HAS NO ANSWERS
L2 STR



G1 C,N
G2 O,N

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 15:13:13 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 130 TO ITERATE

100.0% PROCESSED 130 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH **COMPLETE**
PROJECTED ITERATIONS: 1916 TO 3284
PROJECTED ANSWERS: 6 TO 266

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L3             6 SEA SSS SAM L1

=> s l1 sss ful
FULL SEARCH INITIATED 15:13:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     2611 TO ITERATE

100.0% PROCESSED     2611 ITERATIONS                                157 ANSWERS
SEARCH TIME: 00.00.01

L4           157 SEA SSS FUL L1

=> s l2 sub=l4 sss ful
FULL SUBSET SEARCH INITIATED 15:13:27 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -       80 TO ITERATE

100.0% PROCESSED       80 ITERATIONS                                 54 ANSWERS
SEARCH TIME: 00.00.01

L5            54 SEA SUB=L4 SSS FUL L2

=> fil cap
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     238.51     238.73

FILE 'CAPLUS' ENTERED AT 15:13:34 ON 21 APR 2010
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FILE LAST UPDATED: 20 Apr 2010  (20100420/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED:  Feb 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE:  Feb 2010

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the first quarter of 2010.

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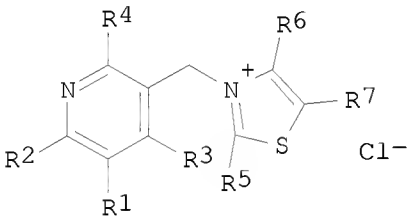
This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l4
L6            37 L4

=> s l5
L7            15 L5
```

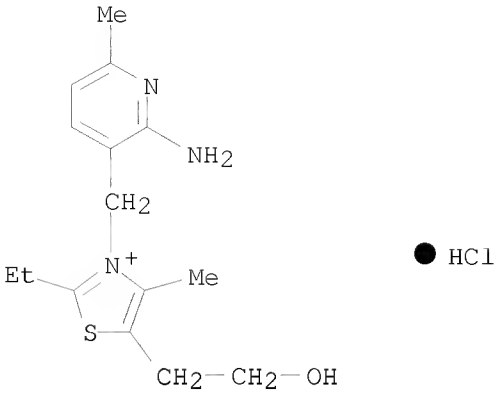
=> d l7 ibib abs hitstr

L7 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:338628 CAPLUS
DOCUMENT NUMBER: 148:561774
TITLE: Synthesis, in vitro and in vivo activity of thiamine antagonist transketolase inhibitors
AUTHOR(S): Thomas, Allen A.; Le Huerou, Y.; De Meese, J.; Gunawardana, Indrani; Kaplan, Tomas; Romoff, Todd T.; Gonzales, Stephen S.; Condroski, Kevin; Boyd, Steven A.; Ballard, Josh; Bernat, Bryan; DeWolf, Walter; Han, May; Lee, Patrice; Lemieux, Christine; Pedersen, Robin; Pheneger, Jed; Poch, Greg; Smith, Darin; Sullivan, Francis; Weiler, Solly; Wright, S. Kirk; Lin, Jie; Brandhuber, Barb; Vigers, Guy
CORPORATE SOURCE: Array BioPharma Inc., Boulder, CO, 80301, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2008), 18(6), 2206-2210
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:561774
GI

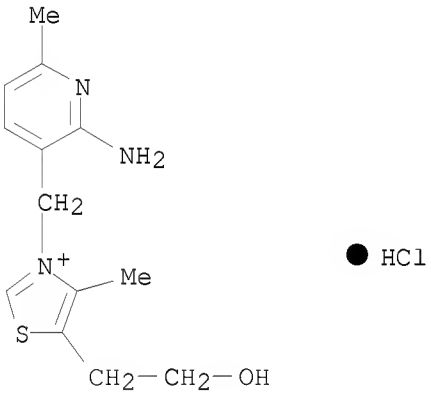


I

AB Transketolase is a key enzyme in the pentose phosphate pathway, which is extensively utilized by tumor cells for the synthesis of ribose, and has been suggested as a target for inhibition in the treatment of cancer. In a pharmacodynamic study, nude mice with xenografted HCT-116 tumors were dosed with I (R1 = R3 = R5 = H; R2 = R6 = Me; R4 = NH2; R7 = CH2CH2OH), an analog of thiamine, the co-factor of transketolase. Transketolase activity was almost completely suppressed in blood, spleen, and tumor cells, but there was little effect on the activity of the other thiamine-utilizing enzymes α-ketoglutarate dehydrogenase or glucose-6-phosphate dehydrogenase. Synthesis and SAR of transketolase inhibitors I (R1 = H, Me; R2 = H, Cl, Me, CF3, NH2, Et, CN, AcNH; R3 = H, Me, NH2, CF3; R4 = H, NH2; R5 = H, Me, Et, CHMeOH, etc.; R6 = H, Me, Et, CH2OH; R7 = CH2CH2OH, CH(OH)CH2OH, CH2CH2CN, etc.) is described.
IT 1026039-14-4P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(docking studies; synthesis and in vitro and in vivo activity of thiamine antagonist transketolase inhibitors)
RN 1026039-14-4 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-2-ethyl-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



IT 13860-66-7P
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and in vitro and in vivo activity of thiamine antagonist transketolase inhibitors)
RN 13860-66-7 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



IT 109402-01-9P 866561-94-6P 1026038-70-9P
1026038-73-2P 1026038-76-5P 1026038-77-6P
1026038-92-5P 1026038-93-6P 1026038-96-9P
1026038-99-2P 1026039-06-4P 1026039-08-6P
1026039-09-7P 1026039-17-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and in vitro and in vivo activity of thiamine antagonist transketolase inhibitors)
RN 109402-01-9 CAPLUS

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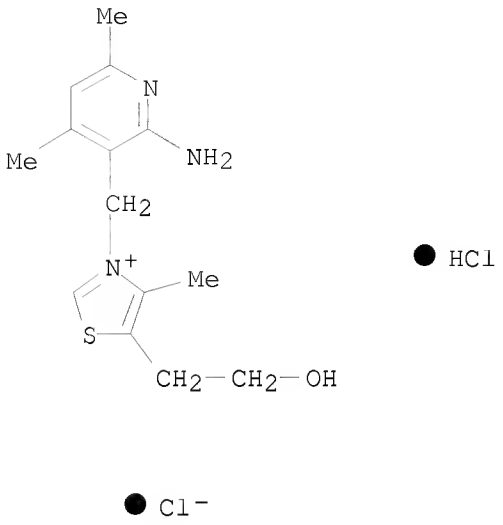

RN 866561-94-6 CAPLUS
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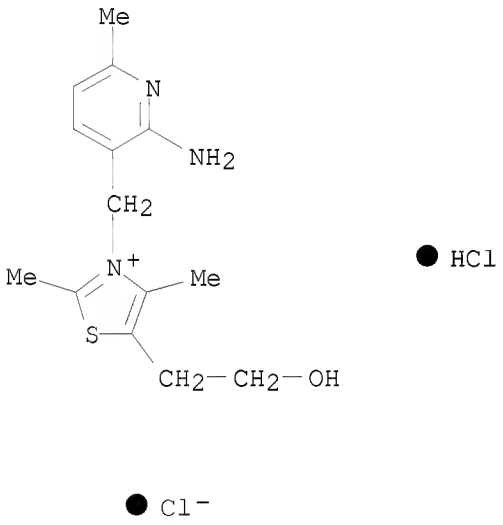

RN 1026038-70-9 CAPLUS
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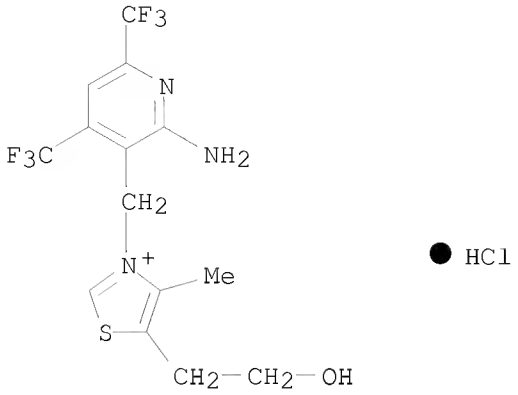

RN 1026038-73-2 CAPLUS
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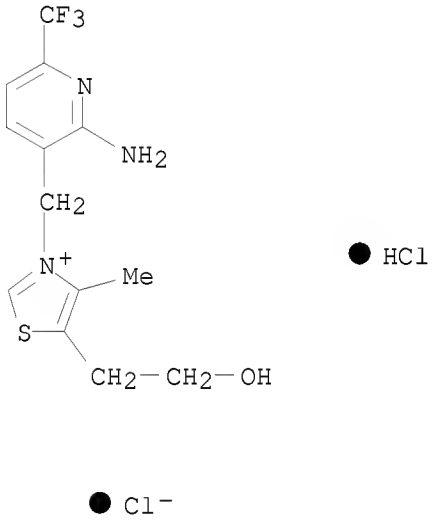

RN 1026038-76-5 CAPLUS
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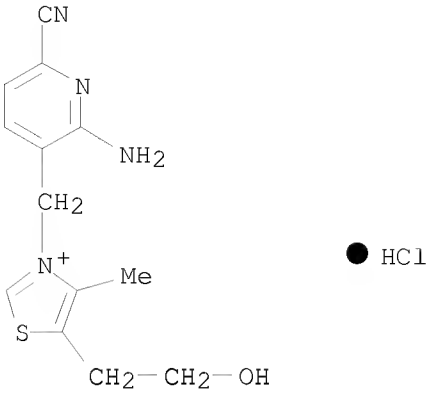

● HCl

RN 1026038-77-6 CAPLUS
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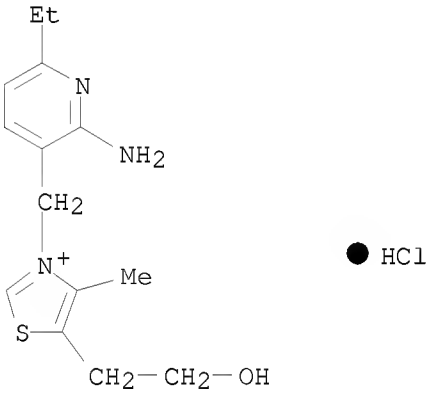

● HCl

RN 1026038-92-5 CAPLUS
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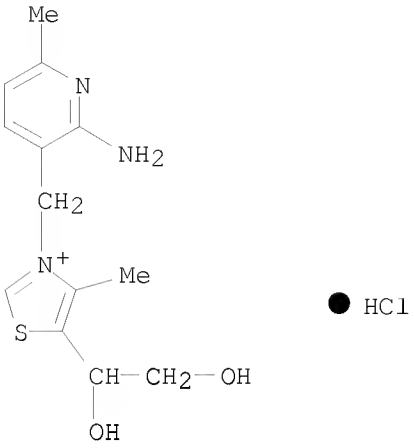

RN 1026038-93-6 CAPLUS
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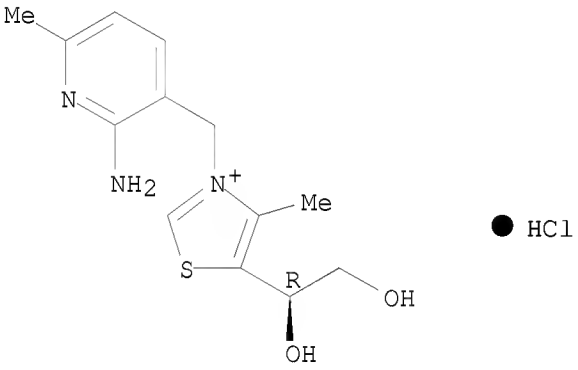
Absolute stereochemistry.



RN 1026038-96-9 CAPLUS
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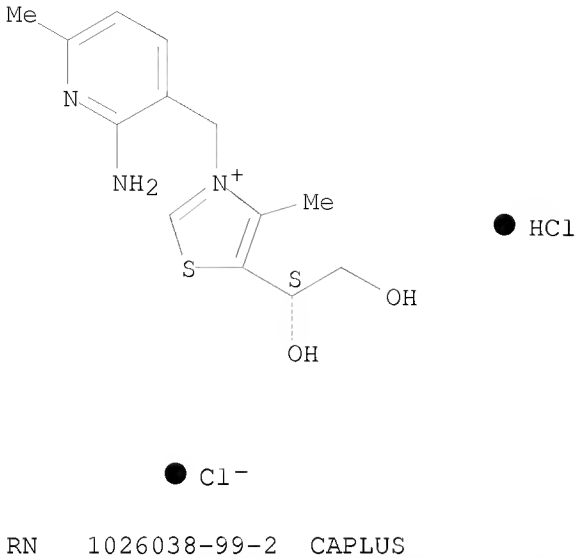
Absolute stereochemistry.



RN 1026038-99-2 CAPLUS
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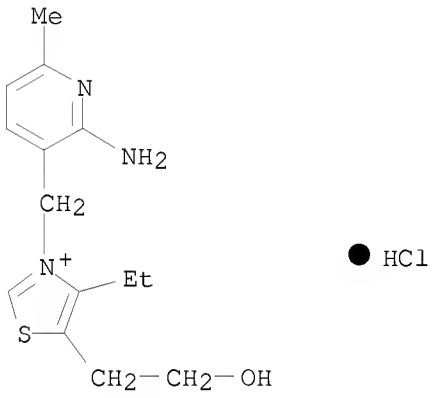

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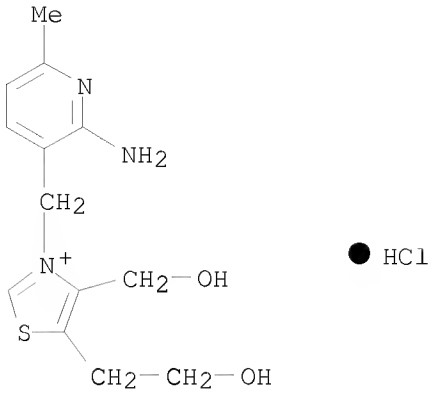

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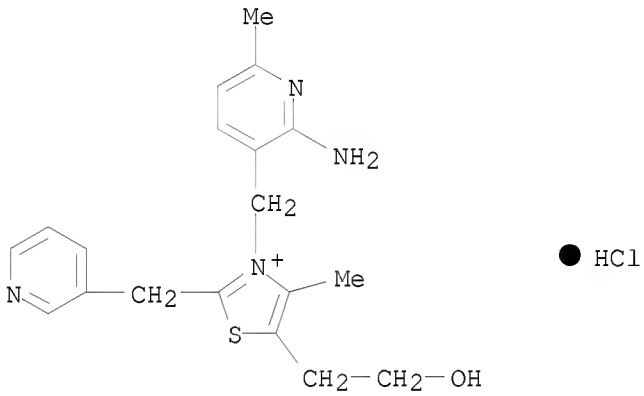

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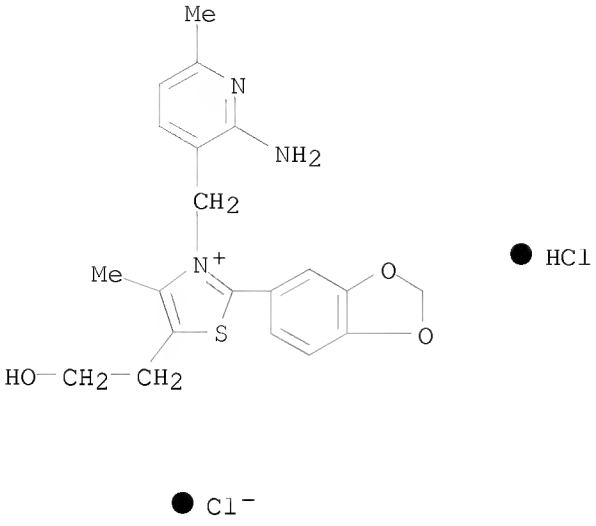

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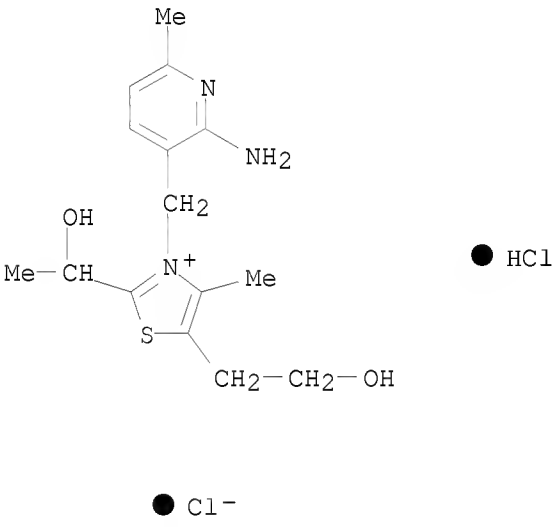

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REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d l7 ibib abs hitstr tot

L7 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:338628 CAPLUS
DOCUMENT NUMBER: 148:561774
TITLE: Synthesis, in vitro and in vivo activity of thiamine antagonist transketolase inhibitors
AUTHOR(S): Thomas, Allen A.; Le Huerou, Y.; De Meese, J.; Gunawardana, Indrani; Kaplan, Tomas; Romoff, Todd T.;

Gonzales, Stephen S.; Condroski, Kevin; Boyd, Steven A.; Ballard, Josh; Bernat, Bryan; DeWolf, Walter; Han, May; Lee, Patrice; Lemieux, Christine; Pedersen, Robin; Pheneger, Jed; Poch, Greg; Smith, Darin; Sullivan, Francis; Weiler, Solly; Wright, S. Kirk; Lin, Jie; Brandhuber, Barb; Vigers, Guy
CORPORATE SOURCE: Array BioPharma Inc., Boulder, CO, 80301, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2008), 18(6), 2206-2210
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:561774
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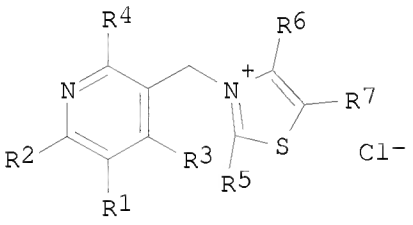
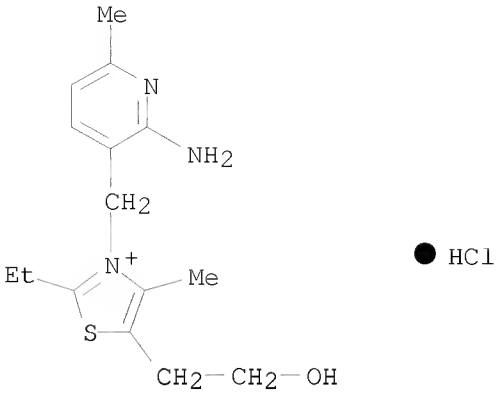
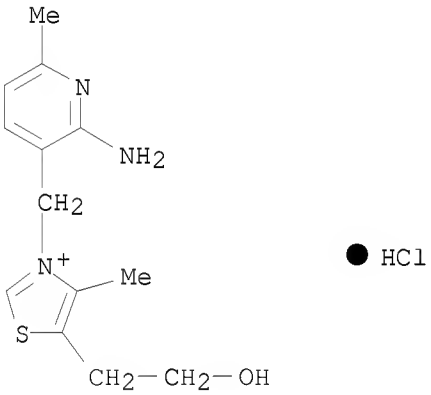


I

AB Transketolase is a key enzyme in the pentose phosphate pathway, which is extensively utilized by tumor cells for the synthesis of ribose, and has been suggested as a target for inhibition in the treatment of cancer. In a pharmacodynamic study, nude mice with xenografted HCT-116 tumors were dosed with I (R1 = R3 = R5 = H; R2 = R6 = Me; R4 = NH2; R7 = CH2CH2OH), an analog of thiamine, the co-factor of transketolase. Transketolase activity was almost completely suppressed in blood, spleen, and tumor cells, but there was little effect on the activity of the other thiamine-utilizing enzymes α-ketoglutarate dehydrogenase or glucose-6-phosphate dehydrogenase. Synthesis and SAR of transketolase inhibitors I (R1 = H, Me; R2 = H, Cl, Me, CF3, NH2, Et, CN, AcNH; R3 = H, Me, NH2, CF3; R4 = H, NH2; R5 = H, Me, Et, CHMeOH, etc.; R6 = H, Me, Et, CH2OH; R7 = CH2CH2OH, CH(OH)CH2OH, CH2CH2CN, etc.) is described.
IT 1026039-14-4P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(docking studies; synthesis and in vitro and in vivo activity of thiamine antagonist transketolase inhibitors)
RN 1026039-14-4 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-2-ethyl-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)

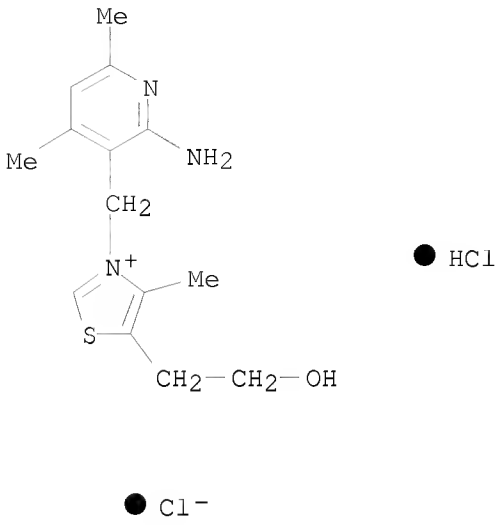


IT 13860-66-7P
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and in vitro and in vivo activity of thiamine antagonist transketolase inhibitors)
RN 13860-66-7 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)

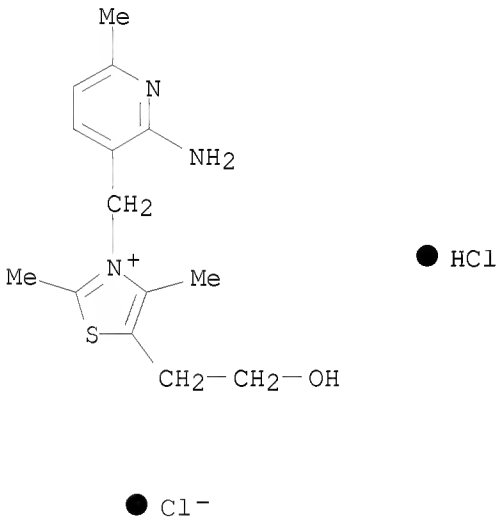


IT 109402-01-9P 866561-94-6P 1026038-70-9P
1026038-73-2P 1026038-76-5P 1026038-77-6P
1026038-92-5P 1026038-93-6P 1026038-96-9P
1026038-99-2P 1026039-06-4P 1026039-08-6P
1026039-09-7P 1026039-17-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and in vitro and in vivo activity of thiamine antagonist transketolase inhibitors)
RN 109402-01-9 CAPLUS

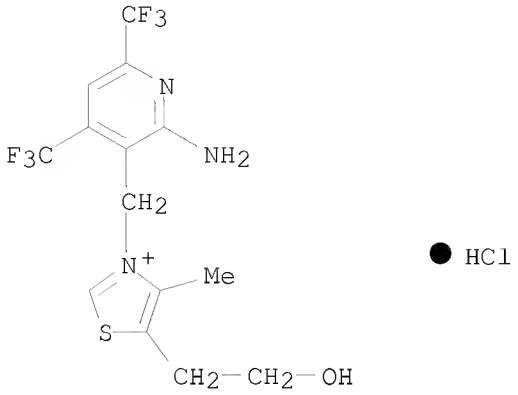
CN Thiazolium, 3-[(2-amino-4,6-dimethyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



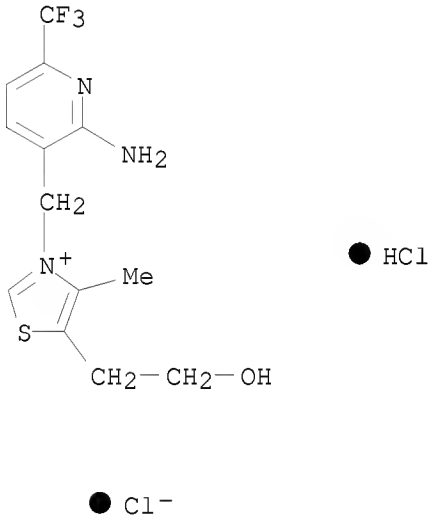
RN 866561-94-6 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-2,4-dimethyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



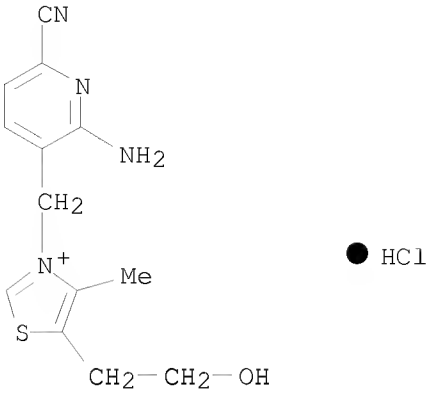
RN 1026038-70-9 CAPLUS
CN Thiazolium, 3-[[2-amino-4,6-bis(trifluoromethyl)-3-pyridinyl]methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



RN 1026038-73-2 CAPLUS
CN Thiazolium, 3-[[2-amino-6-(trifluoromethyl)-3-pyridinyl]methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)

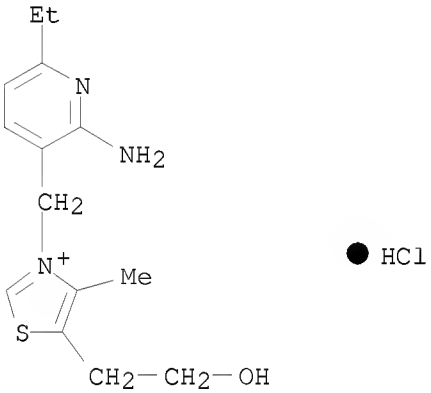


RN 1026038-76-5 CAPLUS
CN Thiazolium, 3-[(2-amino-6-cyano-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



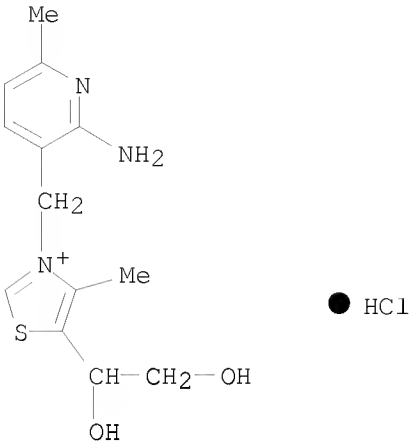
● HCl

RN 1026038-77-6 CAPLUS
CN Thiazolium, 3-[(2-amino-6-ethyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



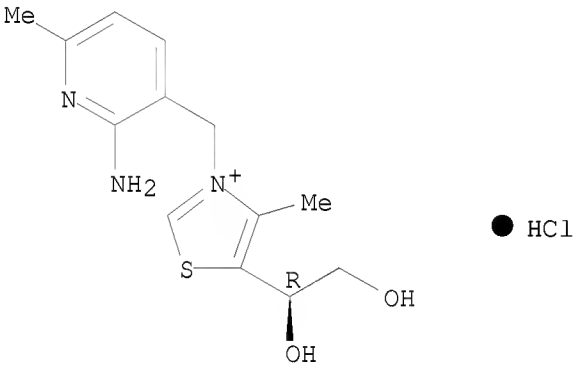
● HCl

RN 1026038-92-5 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(1,2-dihydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



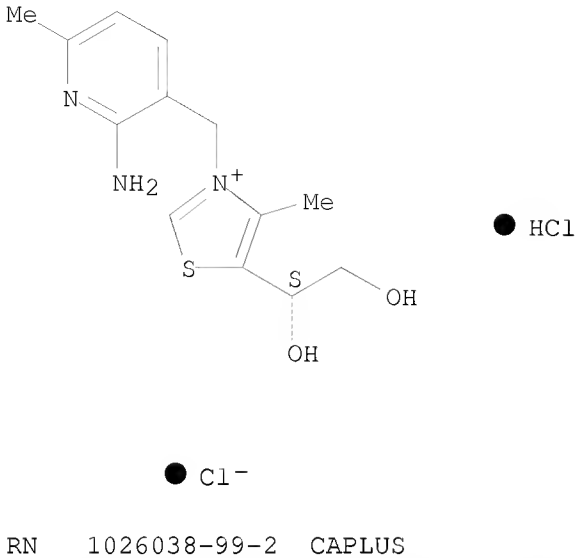
RN 1026038-93-6 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-[(1R)-1,2-dihydroxyethyl]-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)

Absolute stereochemistry.

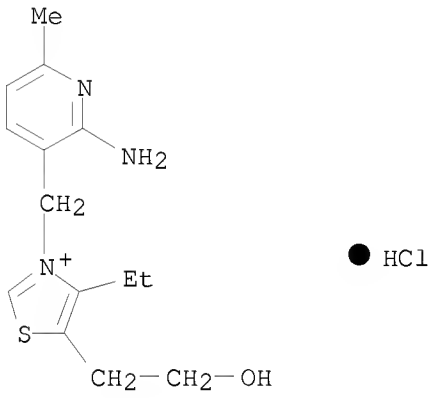


RN 1026038-96-9 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-[(1S)-1,2-dihydroxyethyl]-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)

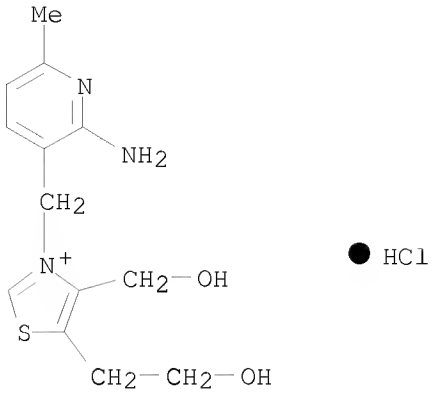
Absolute stereochemistry.



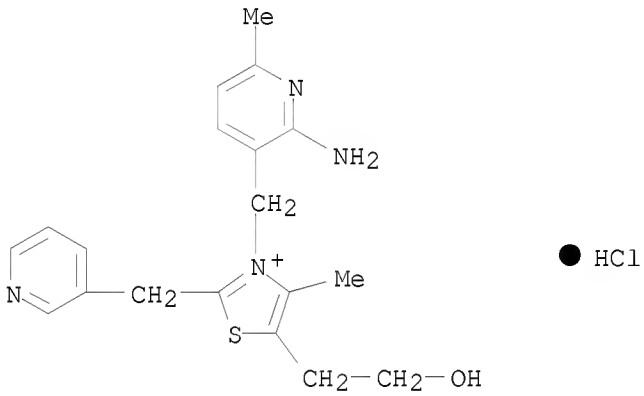
RN 1026038-99-2 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-4-ethyl-5-(2-hydroxyethyl)-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



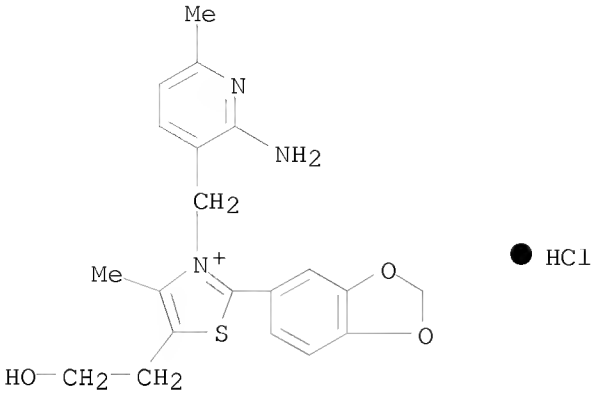
RN 1026039-06-4 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-(hydroxymethyl)-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



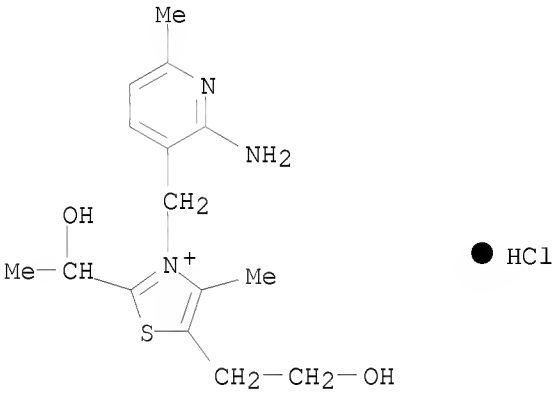
RN 1026039-08-6 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-2-(3-pyridinylmethyl)-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



RN 1026039-09-7 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-2-(1,3-benzodioxol-5-yl)-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



RN 1026039-17-7 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-2-(1-hydroxyethyl)-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



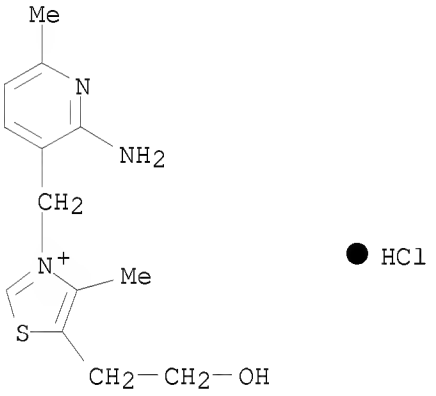
OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:85132 CAPLUS
DOCUMENT NUMBER: 148:345763
TITLE: Non-charged thiamine analogs as inhibitors of enzyme transketolase
AUTHOR(S): Thomas, Allen A.; De Meese, J.; Le Huerou, Y.; Boyd, Steven A.; Romoff, Todd T.; Gonzales, Steven S.; Gunawardana, Indrani; Kaplan, Tomas; Sullivan, Francis; Condroski, Kevin; Lyssikatos, Joseph P.; Aicher, Thomas D.; Ballard, Josh; Bernat, Bryan;

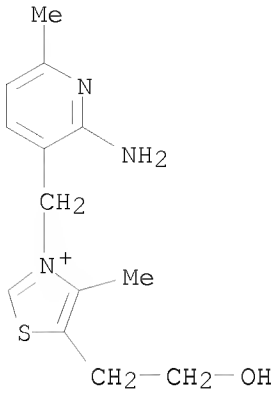
DeWolf, Walter; Han, May; Lemieux, Christine; Smith, Darin; Weiler, Solly; Wright, S. Kirk; Vigers, Guy; Brandhuber, Barb
CORPORATE SOURCE: Array BioPharma Inc., Boulder, CO, 80301, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2008), 18(2), 509-512
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:345763
AB Inhibition of the thiamine-utilizing enzyme transketolase (TK) has been linked with diminished tumor cell proliferation. Most thiamine antagonists have a permanent pos. charge on the B-ring, and it has been suggested that this charge is required for diphosphorylation by thiamine pyrophosphokinase (TPPK) and binding to TK. We sought to make neutral thiazolium replacements that would be substrates for TPPK, while not necessarily needing thiamine transporters (ThTr1 and ThTr2) for cell penetration. The synthesis, SAR, and structure-based rationale for highly potent non-thiazolium TK antagonists are presented.

IT 13860-66-7 866319-88-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(non-charged thiamine analogs preparation as transketolase enzyme inhibitors with better pharmacokinetics)

RN 13860-66-7 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



RN 866319-88-2 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride (1:1) (CA INDEX NAME)



● Cl^-

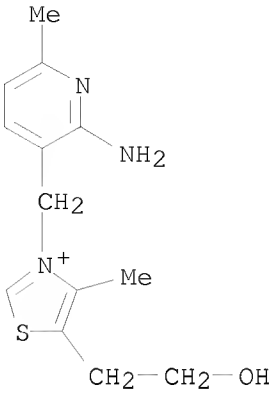
OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

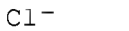
L7 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:85131 CAPLUS
DOCUMENT NUMBER: 148:321825
TITLE: Prodrug thiamine analogs as inhibitors of the enzyme transketolase
AUTHOR(S): Le Huerou, Yvan; Gunawardana, Indrani; Thomas, Allen A.; Boyd, Steven A.; de Meese, Jason; de Wolf, Walter; Gonzales, Steven S.; Han, May; Hayter, Laura; Kaplan, Tomas; Lemieux, Christine; Lee, Patrice; Pheneger, Jed; Poch, Gregory; Romoff, Todd T.; Sullivan, Francis; Weiler, Solly; Wright, S. Kirk; Lin, Jie
CORPORATE SOURCE: Array BioPharma Inc., Boulder, CO, 80301, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2008), 18(2), 505-508
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:321825

AB Transketolase, a key enzyme in the pentose phosphate pathway, has been suggested as a target for inhibition in the treatment of cancer. Compound 5a ('N3'-pyridyl thiamin'; 3-(6-methyl-2-amino-pyridin-3-ylmethyl)-5-(2-hydroxy-ethyl)-4-methyl-thiazol-3-ium chloride hydrochloride), an analog of the transketolase cofactor thiamin, is a potent transketolase inhibitor but suffers from poor pharmacokinetics due to high clearance and Cmax linked toxicity. An efficient way of improving the pharmacokinetic profile of 5a is to prepare oxidized prodrugs which are slowly reduced in vivo yielding longer, sustained blood levels of the drug. The synthesis of such prodrugs and their evaluation in rodent models is reported.

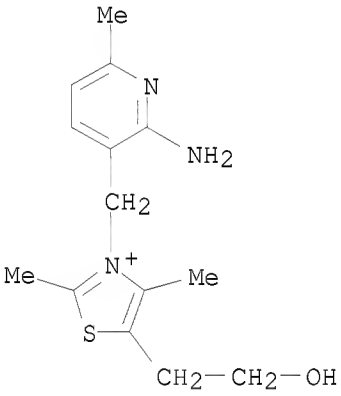
IT 866319-88-2
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(prodrug thiamine analogs as inhibitors of transketolase)

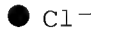
RN 866319-88-2 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride (1:1) (CA INDEX NAME)





IT 866561-30-0
RL: PAC (Pharmacological activity); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(prodrug thiamine analogs as inhibitors of transketolase)
RN 866561-30-0 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-2,4-dimethyl-, chloride (1:1) (CA INDEX NAME)





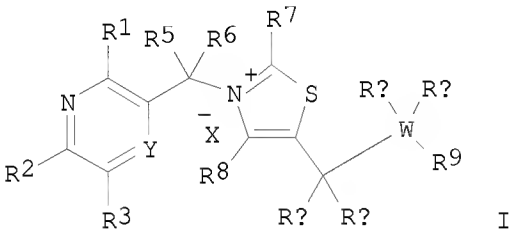
OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)
REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:1106858 CAPLUS
DOCUMENT NUMBER: 143:387024
TITLE: Preparation of pyridylmethyl or pyrazinylmethyl thiazoles as transketolase inhibitors
INVENTOR(S): Boyd, Steven A.

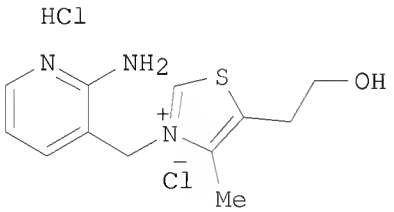
PATENT ASSIGNEE(S): Array Biopharma Inc., USA
SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095391	A1	20051013	WO 2005-US9970	20050323
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20090209554	A1	20090820	US 2008-593910	20080610

PRIORITY APPLN. INFO.: US 2004-556217P P 20040324
WO 2005-US9970 W 20050323
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 143:387024; MARPAT 143:387024
GI



I



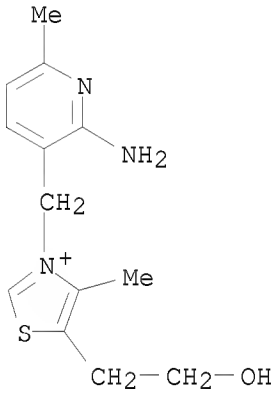
II

AB Title compds. I [Y = N or CR4; W = (C2)n; R1 = H, alkyl, CN, etc.; R2, R3 and R4 independently = H, halo, CN, etc.; R5 and R6 independently = H, alkyl or fluoroalkyl; R7 = H, aralkyl, aryl, etc.; R8 = H, alkyl, heteroaryl, etc.; R9 = OR10 or NR11R12; R10 = heteroaryl, aryl, heterocycle, etc.; R11 = H or alkyl; R12 = H, aralkyl, aryl, etc.; Ra and Rb independently = H, alkyl, fluoroalkyl, etc.; Rc and Rx independently = H, alkyl or fluoroalkyl; n = 0-4; X- = mono- or divalent anion or

counterion to thiazolium nitrogen] and their pharmaceutically acceptable salts, are prepared and disclosed as inhibitors of transketolase inhibitors. Thus, e.g., II was prepared by reduction of 2-aminonicotinic acid using LAH followed by chlorination using SOCl2 and subsequent substitution with 2-(4-methylthiazol-5-yl)ethanol. The ability of I to be phosphorylated by thiamine pyrophosphate kinase 1 (TPK1) was evaluated and it was revealed that selected compds. of the invention possessed IC50 values in the range of 8.83 up to 851 nM. I as transketolase inhibitors should prove useful in the treatment of neoplasm. Pharmaceutical compns. comprising I are disclosed.

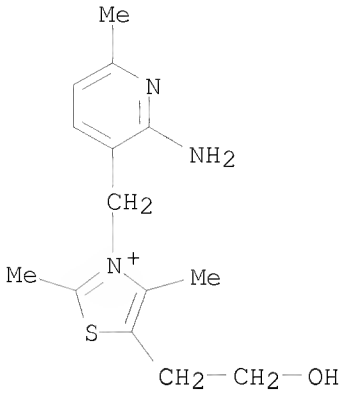
IT 866319-88-2P 866561-30-0P 866561-53-7P
866561-67-3P 866561-68-4P 866561-69-5P
866561-73-1P 866561-74-2P 866561-75-3P
866561-76-4P 866561-77-5P 866561-78-6P
866561-79-7P 866561-80-0P 866561-81-1P
866561-82-2P 866561-94-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyridylmethyl or pyrazinylmethyl thiazoles as transketolase inhibitors)

RN 866319-88-2 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride (1:1) (CA INDEX NAME)

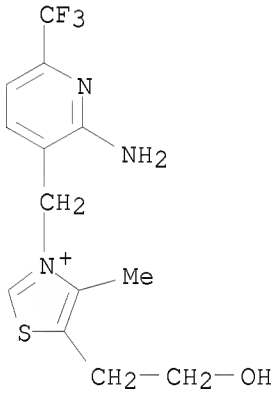


● Cl⁻

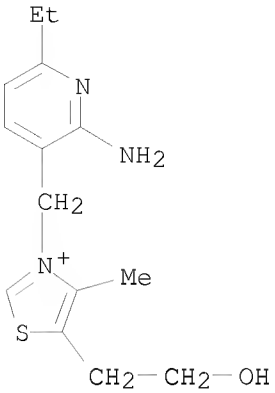
RN 866561-30-0 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-2,4-dimethyl-, chloride (1:1) (CA INDEX NAME)



RN 866561-53-7 CAPLUS
CN Thiazolium, 3-[[2-amino-6-(trifluoromethyl)-3-pyridinyl]methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride (1:1) (CA INDEX NAME)

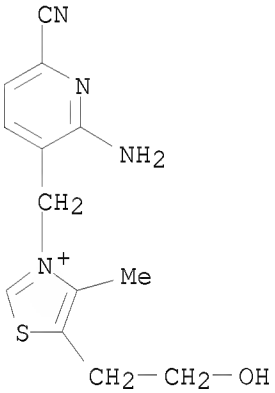


RN 866561-67-3 CAPLUS
CN Thiazolium, 3-[(2-amino-6-ethyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride (1:1) (CA INDEX NAME)



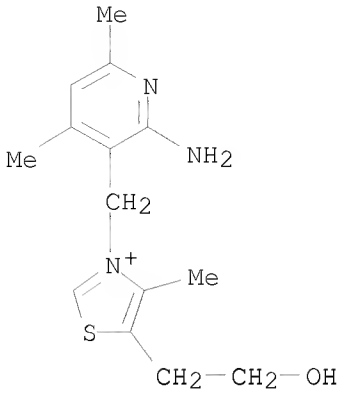
● Cl^-

RN 866561-68-4 CAPLUS
CN Thiazolium, 3-[(2-amino-6-cyano-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride (1:1) (CA INDEX NAME)



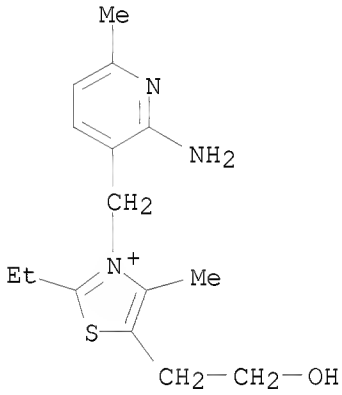
● Cl^-

RN 866561-69-5 CAPLUS
CN Thiazolium, 3-[(2-amino-4,6-dimethyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride (1:1) (CA INDEX NAME)



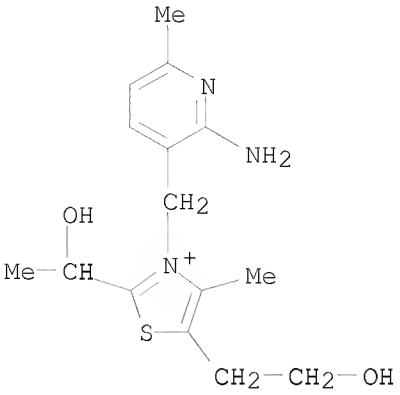
● Cl^-

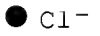
RN 866561-73-1 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-2-ethyl-5-(2-hydroxyethyl)-4-methyl-, chloride (1:1) (CA INDEX NAME)



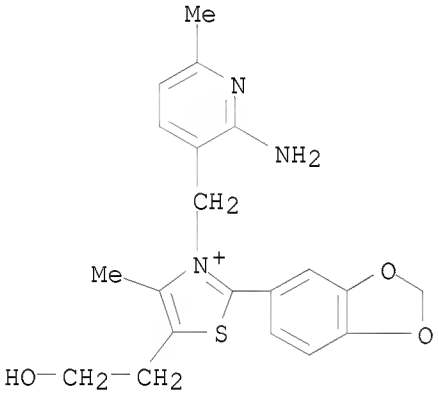
● Cl^-

RN 866561-74-2 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-2-(1-hydroxyethyl)-5-(2-hydroxyethyl)-4-methyl-, chloride (1:1) (CA INDEX NAME)

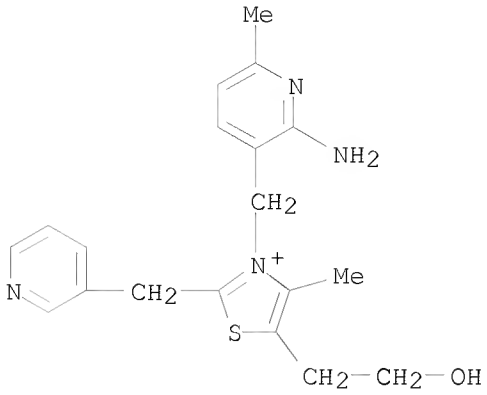




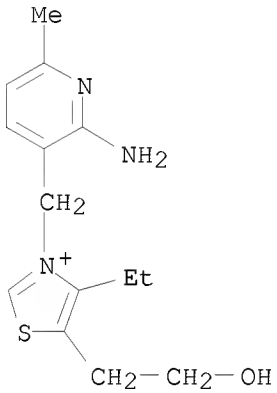
RN 866561-75-3 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-2-(1,3-benzodioxol-5-yl)-5-(2-hydroxyethyl)-4-methyl-, chloride (1:1) (CA INDEX NAME)



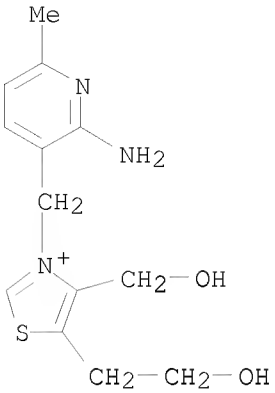
RN 866561-76-4 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-2-(3-pyridinylmethyl)-, chloride (1:1) (CA INDEX NAME)



RN 866561-77-5 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-4-ethyl-5-(2-hydroxyethyl)-, chloride (1:1) (CA INDEX NAME)

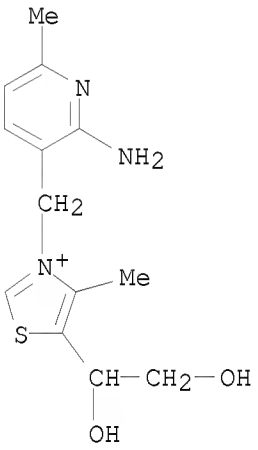


RN 866561-78-6 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-(hydroxymethyl)-, chloride (1:1) (CA INDEX NAME)



● Cl^-

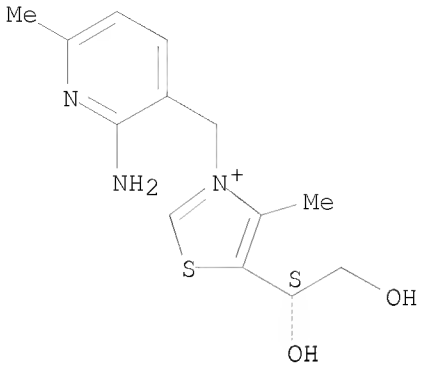
RN 866561-79-7 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(1,2-dihydroxyethyl)-4-methyl-, chloride (1:1) (CA INDEX NAME)



● Cl^-

RN 866561-80-0 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-[(1S)-1,2-dihydroxyethyl]-4-methyl-, chloride (1:1) (CA INDEX NAME)

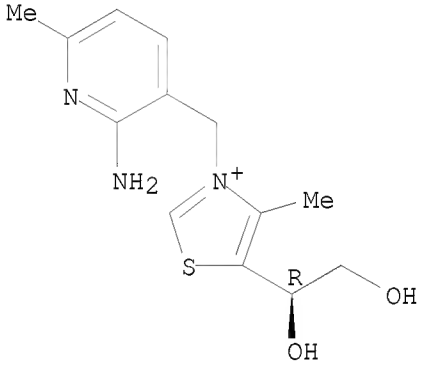
Absolute stereochemistry.



● Cl^-

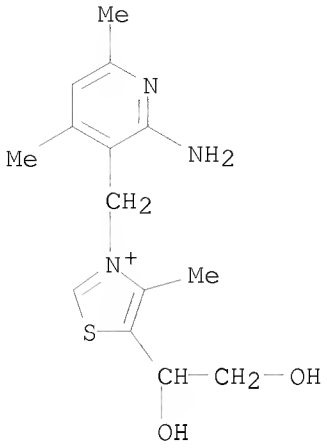
RN 866561-81-1 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-[(1R)-1,2-dihydroxyethyl]-4-methyl-, chloride (1:1) (CA INDEX NAME)

Absolute stereochemistry.

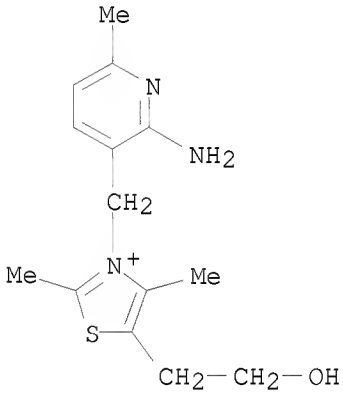


● Cl^-

RN 866561-82-2 CAPLUS
CN Thiazolium, 3-[(2-amino-4,6-dimethyl-3-pyridinyl)methyl]-5-(1,2-dihydroxyethyl)-4-methyl-, chloride (1:1) (CA INDEX NAME)



RN 866561-94-6 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-2,4-dimethyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:1103891 CAPLUS
DOCUMENT NUMBER: 143:381795
TITLE: Fluorescence assay for measuring activities of thiamine pyrophosphate-dependent enzymes in cells, blood, tumors, and tissues, and use in drug dosing and discovery
INVENTOR(S): Han, May
PATENT ASSIGNEE(S): Genpath Pharmaceuticals, Inc., USA; Aveo

Pharmaceuticals, Inc.
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095636	A2	20051013	WO 2005-US9759	20050323
WO 2005095636	A3	20060427		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20070292888	A1	20071220	US 2007-594194	20070427

PRIORITY APPLN. INFO.:			
US 2004-556281P	P	20040324	
WO 2005-US9759	W	20050323	

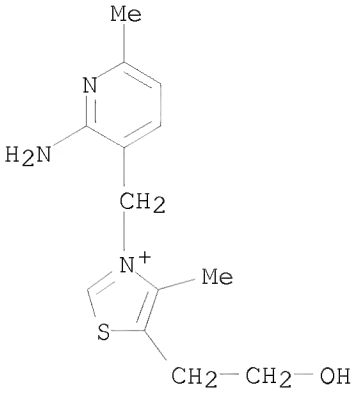
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

AB The invention provides improved and high through-put methods for measuring enzymic activities involved in the oxidative and non-oxidative pentose phosphate pathways, and other thiamine pyrophosphate containing enzymes, which are commonly elevated in tumor cells. The invention provides improved methods for measuring transketolase, α-ketoglutarate dehydrogenase, pyruvate dehydrogenase, and glucose-6-phosphate dehydrogenase activities in cultured cells, blood, tumors and other tissues using the step of monitoring production of NADH or NADPH by fluorescence. The increased sensitivity of this fluorescence assay, which can be performed on cell lysates, significantly improves the assays of the present invention over enzymic assays that monitor absorption. The assays of the invention are useful for optimizing therapeutic dosing and scheduling of drugs acting on the pentose phosphate pathways by sampling and monitoring enzymic levels in a treated patient over time. Finally, the assays are useful for drug discovery, as well as for preclin. and clin. development of anti-cancer therapeutics and for determining drug dosing and scheduling in the clinic.

IT 13857-23-3
RL: BSU (Biological study, unclassified); BIOL (Biological study) (comparison of inhibition by N3PT with inhibition by TPP mimetic drug; fluorescence assay for measuring activities of thiamine pyrophosphate-dependent enzymes in cells, blood, tumors, and tissues, and use in drug dosing and discovery)

RN 13857-23-3 CAPLUS

CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl- (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:1103748 CAPLUS
DOCUMENT NUMBER: 143:386689
TITLE: Preparation of thioalkeneamides as transketolase inhibitors
INVENTOR(S): Boyd, Steven A.
PATENT ASSIGNEE(S): Array Biopharma Inc., USA
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095344	A1	20051013	WO 2005-US9966	20050323
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20070293501	A1	20071220	US 2007-593911	20070511
PRIORITY APPLN. INFO.:			US 2004-556218P P	20040324
			WO 2005-US9966 W	20050323

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 143:386689; MARPAT 143:386689
GI

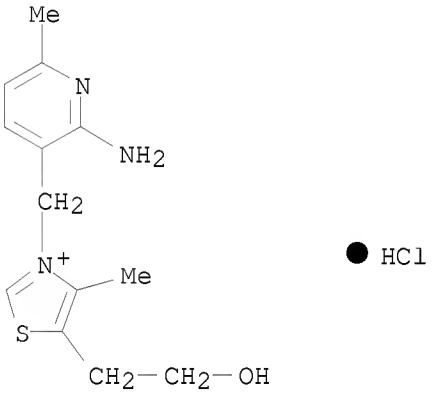
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [A = pyridinyl or pyrazinyl; R1 and R2 independently = H, alkyl or fluoroalkyl; R3 = H, heterocycle, aryl, etc.; R4 = H, alkyl,

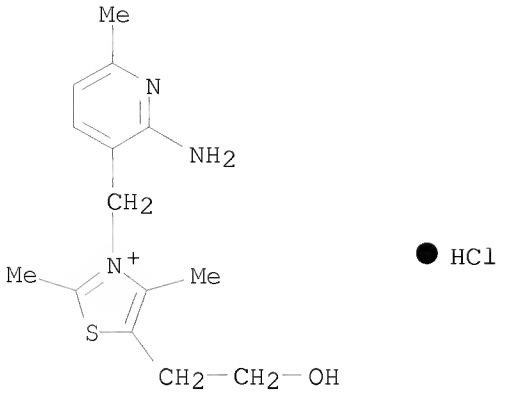
fluoroalkyl, etc.; R5 = OR7 or NR8R9; R6 = C(O)R, C(S)R, SR, etc.; R7 = C(O)NR2, C(O)OR, (CH2)1-6-C(O)R, etc.; Ra and Rb independently = H, alkyl, fluoroalkyl, etc.; Rc and Rx independently = H, alky or fluoroalkyl; n = 0-4; R = carbocycle, aryl, heteroaryl, etc.] and their pharmaceutically acceptable salts, are prepared and disclosed as inhibitors of transketolase inhibitors. Thus, e.g., II was prepared by coupling of 2-(4-methylthiazol-5-yl)ethanol with 3-chloromethyl-6-methylpyridin-2-ylamine hydrochloride (preparation given) and subsequent ring opening and disulfide bridge formation using potassium ferricyanide. The ability of I to be phosphorylated by thiamine pyrophosphate kinase 1 (TPK1) was evaluated and it was revealed that selected compds. of the invention possessed IC50 values in the range of 10.13 up to 803.23 nM. I as transketolase inhibitors should prove useful in the treatment of neoplasm. Pharmaceutical compns. comprising I are disclosed.

IT 13860-66-7P 866561-94-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of thioalkeneamides as transketolase inhibitors)

RN 13860-66-7 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



RN 866561-94-6 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-2,4-dimethyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)

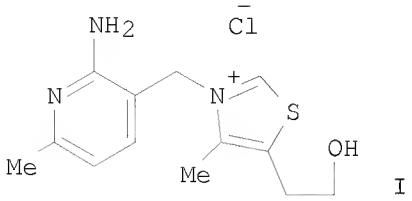


REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:1103561 CAPLUS
DOCUMENT NUMBER: 143:360092
TITLE: N3-pyridylthiamine and its use in cancer treatment
INVENTOR(S): Gyuris, Jeno; O'Hagan, Ronan C.; Han, May; Robinson, Murray; Weiler, Solly
PATENT ASSIGNEE(S): Genpath Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005094803	A2	20051013	WO 2005-US9758	20050323
WO 2005094803	A3	20051201		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20080234304	A1	20080925	US 2008-594191	20080429

PRIORITY APPLN. INFO.: US 2004-556219P P 20040324
WO 2005-US9758 W 20050323
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
GI



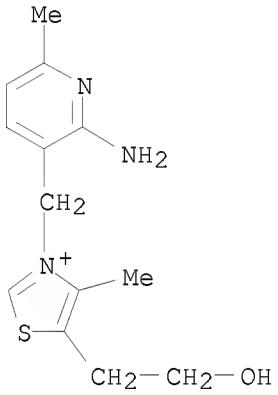
I

AB The invention provides methods using N3-pyridylthiamine (I) and pharmaceutical compns. comprising N3-pyridylthiamine, which are especially useful for preventing or reducing tumor growth in vivo. The invention is also directed to the benefits of reducing thiamine concns., e.g., by means of a thiamine-reduced diet, as an effective step in a therapeutic regime for patients treated with N3-pyridylthiamine.

IT 866319-88-2 866319-88-2D, conjugates
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(N3-pyridylthiamine for cancer treatment)

RN 866319-88-2 CAPLUS

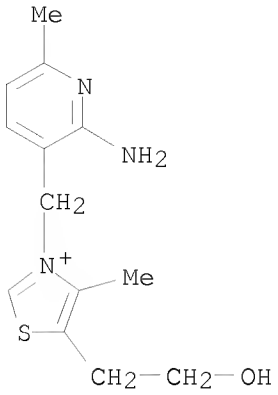
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride (1:1) (CA INDEX NAME)



● Cl^-

RN 866319-88-2 CAPLUS

CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride (1:1) (CA INDEX NAME)



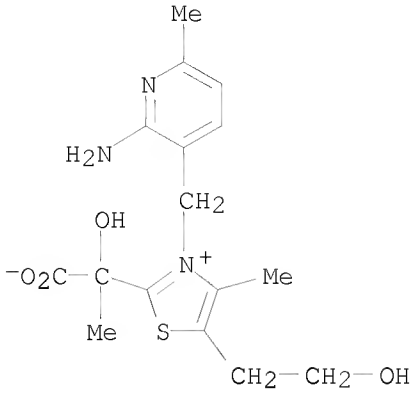
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L7 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1994:649197 CAPLUS
DOCUMENT NUMBER: 121:249197
ORIGINAL REFERENCE NO.: 121:45399a,45402a
TITLE: Theoretical studies on thiamin-substrate adducts
AUTHOR(S): Friedemann, R.; Breitkopf, C.
CORPORATE SOURCE: Dep. Phys. Chem., Martin Luther Univ., Halle/Saale, 06108, Germany
SOURCE: Bioorganic Chemistry (1994), 22(2), 119-27
CODEN: BOCMBM; ISSN: 0045-2068
DOCUMENT TYPE: Journal
LANGUAGE: English

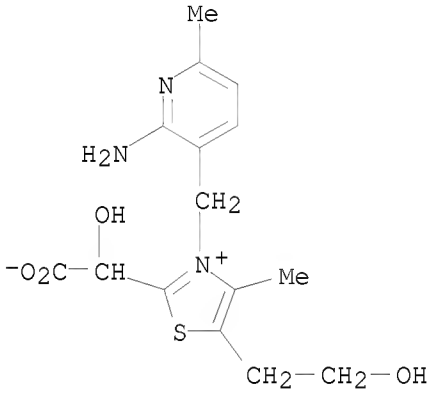
AB The conformational behavior and stability of thiamin adducts formed by the C2 addition of the substrates pyruvate and glyoxylate to the thiamin system as well as its decarboxylation products are investigated within the force field version PIMM90 and the semiempirical PM3 method. The calcns. on the key intermediates of the Breslow mechanism are performed to study the steric aspects of both adducts which show a different pathway in the catalytic cycle. Moreover, the energetic and steric influence of the 5'-aminopyrimidine ring on the generation of the relevant conformations of the intermediates is taken into account. The most stable conformers of the adducts are characterized by V-like structures and the formation of a significant intramol. hydrogen bonding under participation of the 4'-amino group. The findings support the "least-motion-maximum-overlap mechanism" and the relay function of the substituted pyrimidine ring. The calcns. on the decarboxylation products of both adducts show that the energetically preferred structure essentially corresponds to an enamine resonance contributor in comparison with the α-carbanion resonance. There are no hints for a different stabilization of the intermediates of both substrate adducts by steric reasons within the simple nonenzymic model.

IT 158498-25-0 158498-26-1 158498-27-2
158498-28-3
RL: PRP (Properties)
(conformation of, theor. study of)

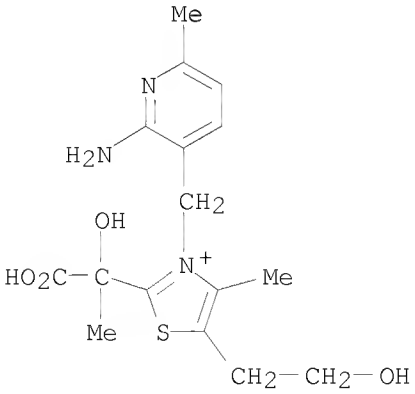
RN 158498-25-0 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-2-(1-carboxy-1-hydroxyethyl)-5-(2-hydroxyethyl)-4-methyl-, inner salt (CA INDEX NAME)



RN 158498-26-1 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-2-(carboxyhydroxymethyl)-5-(2-hydroxyethyl)-4-methyl-, inner salt (CA INDEX NAME)

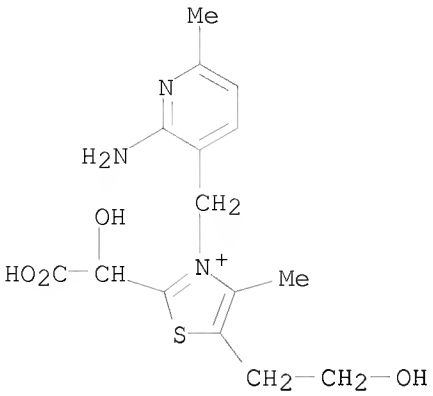


RN 158498-27-2 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-2-(1-carboxy-1-hydroxyethyl)-5-(2-hydroxyethyl)-4-methyl- (CA INDEX NAME)



RN 158498-28-3 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-2-

(carboxyhydroxymethyl)-5-(2-hydroxyethyl)-4-methyl- (CA INDEX NAME)

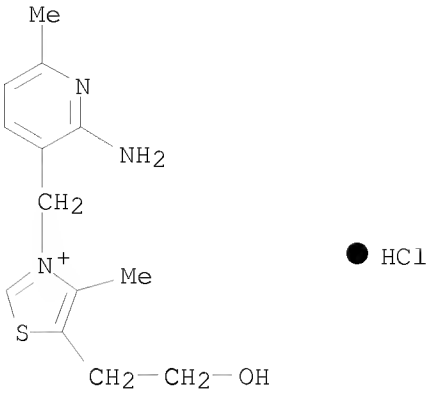


OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

L7 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1989:627877 CAPLUS
DOCUMENT NUMBER: 111:227877
ORIGINAL REFERENCE NO.: 111:37761a,37764a
TITLE: 4'-N-dimethyl-, N-1'-, and N-3'-pyridylthiamin diphosphate coenzyme function in a transketolase-catalyzed reaction
AUTHOR(S): Meshalkina, L. E.; Golbik, R.; Usmanov, R. A.; Neef, H.; Schellenberger, A.; Kochetov, G. A.
CORPORATE SOURCE: Mosk. Gos. Univ., Moscow, USSR
SOURCE: Doklady Akademii Nauk SSSR (1989), 307(2), 486-90 [Biochem.]
CODEN: DANKAS; ISSN: 0002-3264
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB The mechanism of the transketolase (EC 2.2.1.1) reaction was examined by studying the interaction of the enzyme with 3 coenzyme analogs (4'-N-dimethyl, N-1'-, and N-3'-pyridylthiamin diphosphate). The 4'-N-dimethylthiamin diphosphate analog inhibited the 2 enzyme active sites with Ki values of 3 and 10 μM. The Km values for thiamin diphosphate were 0.03 and 0.5 μM. The N-1'-pyridylthiamin diphosphate analog displayed nearly identical Km values (0.08 and 0.4 μM), demonstrating that the N-1'-pyridyl group was not involved in binding to the enzyme. The N-3'-pyridylthiamin diphosphate analog displayed a Ki value for each active site of 1.3 nM.

IT 13860-66-7
RL: BIOL (Biological study)
(transketolase inhibition by, kinetics of)
RN 13860-66-7 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)

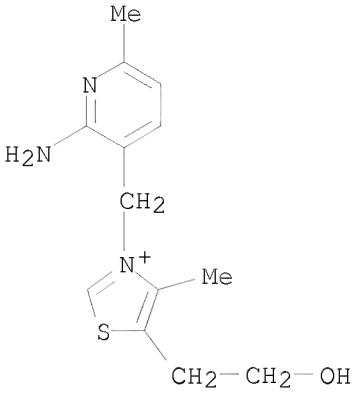


OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

L7 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1977:529453 CAPLUS
DOCUMENT NUMBER: 87:129453
ORIGINAL REFERENCE NO.: 87:20557a,20560a
TITLE: Interaction of thiamin analogs with yeast thiamin pyrophosphokinase
AUTHOR(S): Ostrovskii, Yu. M.; Chernikevich, I. P.; Voskoboev, A. I.; Shellenberger, A.
CORPORATE SOURCE: Metab. Regul. Div., Grodno, USSR
SOURCE: Bioorganicheskaya Khimiya (1977), 3(8), 1083-9
CODEN: BIKHD7; ISSN: 0132-3423
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB The phosphorylation of various thiamin derivs. by yeast thiamin pyrophosphokinase (EC 2.7.6.2) was studied. Some thiamin analogs substituted in the 2'-position of the pyrimidine ring were more effectively phosphorylated than thiamin, and removal or modification of the heterocyclic amino groups did not result in decreased interaction with the kinase. Substitution of Me or Et radicals in the 6'-position or substitution of 1'-N or 3'-N with CH did not significantly affect the rate of enzyme reaction. The interconversion between thiol-disulfide groups in the thiazole ring did not have any direct relation with thiamin binding by the kinase. The most important groups for interaction of substrate with kinase appear to be the quaternary N atom and the 5-hydroxyethyl radical.

IT 13857-23-3
RL: BIOL (Biological study)
(thiamin pyrophosphokinase specificity for)
RN 13857-23-3 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl- (CA INDEX NAME)

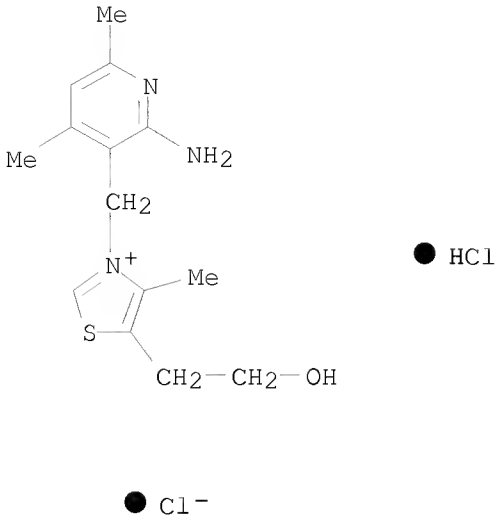


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L7 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1958:103658 CAPLUS
DOCUMENT NUMBER: 52:103658
ORIGINAL REFERENCE NO.: 52:18170i,18171a
TITLE: Preparation of a surface layer of an alloy on metals
INVENTOR(S): Franssen, Hermann
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 865407		19530202	DE 1951-F6360	19510605

AB A layer of a protective alloy having a comparatively high vapor pressure is formed on the surface of a metal having a low vapor pressure by heating at 700-850° the metal to be alloyed, such as Cu, with a metal of a higher vapor pressure, such as Zn, in the presence of a reductive protective gas.
IT 109402-01-9
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 109402-01-9 CAPLUS
CN Thiazolium, 3-[(2-amino-4,6-dimethyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



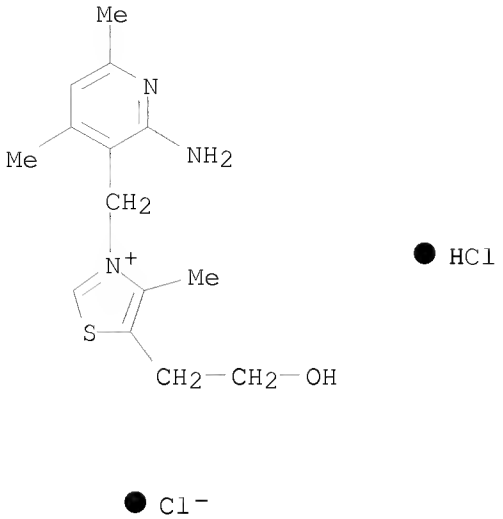
L7 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1958:103657 CAPLUS
DOCUMENT NUMBER: 52:103657
ORIGINAL REFERENCE NO.: 52:18170h-i
TITLE: Measuring the content of alloy components in metal melts
INVENTOR(S): Beilfuss, Siegfried
PATENT ASSIGNEE(S): Deutsche Bundesbahn
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 865380		19530202	DE 1951-D8677	19510415

AB The content of the respective components in an alloy melt is measured by determining the sp. weight of the components by use of an aerometer which is filled with a metal corresponding to the heaviest metal contained in the alloy and which is immersed in the fluid metal. The aerometer is provided with a heat-resistant covering and contains a calibrated spindle whose expansion or contraction depends on the heat-expansion coefficient of the metal.

IT 109402-01-9
(Derived from data in the 6th Collective Formula Index (1957-1961))

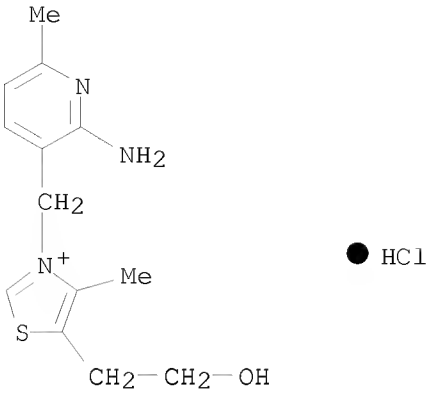
RN 109402-01-9 CAPLUS
CN Thiazolium, 3-[(2-amino-4,6-dimethyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)

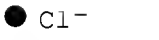


L7 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1957:100344 CAPLUS
DOCUMENT NUMBER: 51:100344
ORIGINAL REFERENCE NO.: 51:18170g-i,18171a
TITLE: Action of two Dornow vitamin B1 analogs and their antagonists in pigeons
AUTHOR(S): Schennert, Arthur; Haenel, Helmut
CORPORATE SOURCE: Vitamin Research Inst., Potsdam-Rehbrucke, Germany
SOURCE: Hoppe-Seyler's Zeitschrift fuer Physiologische Chemie (1953), 295, 354-62
CODEN: HSZPAZ; ISSN: 0018-4888
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

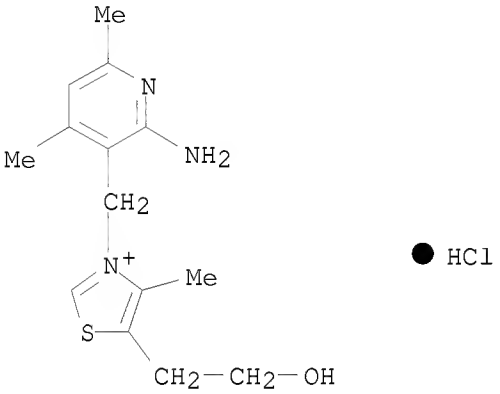
AB cf. Dornow and Hargesheimer, C.A. 49, 3200c. The activity of 2 vitamin B1 analogs and their antivitamins was determined by using a pigeon test. In one the pyrimidine ring was replaced also by a pyridine ring. The following compds. were tested: 4-methyl-5-(2-hydroxyethyl)-N-(2-amino-6-methyl-3-pyridylmethyl)thiazolium chloride-HCl, 2-methyl-3-(2-hydroxyethyl)-N-(2-amino-6-methyl-3-pyridylmethyl)-pyridinium chloride-HCl, 4-methyl-5-(2-hydroxyethyl)-N-(2-amino-4,6-dimethyl-3-pyridylmethyl)thiazolium chloride-HCl, and 2-methyl-3-(2-hydroxyethyl)-N-(2-amino-4,6-dimethyl-3 -pyridylmethyl)pyridinium chloride-HCl. Substitution of the pyrimidine ring by 2-amino-6-methyl-3-pyridylmethyl group preserved some vitamin B1 activity. The antivitamin behaved similarly, thereby confirming the theoretical predictions and the microbiol. tests. Introduction of a 4-methyl group in the pyridine ring prevented the pigeon test from being carried out. This does not contradict the weakly pos. result of the microbiol. test, since the pigeon requires correspondingly greater amts. of test substance. It is clear that replacement of the H atoms with Me groups alters the action mechanism of the vitamin B1 analogs.

IT 13860-66-7
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 13860-66-7 CAPLUS
CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)





IT 109402-01-9, 3-[(2-Amino-4,6-dimethyl-3-pyridyl)methyl]-5-(2-hydroxyethyl)-4-methylthiazolium chloride, hydrochloride
(action in pigeons)
RN 109402-01-9 CAPLUS
CN Thiazolium, 3-[(2-amino-4,6-dimethyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



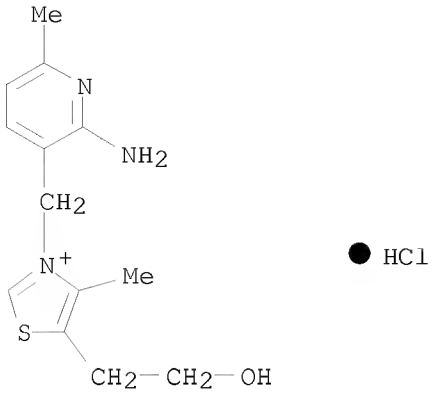
L7 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1955:16062 CAPLUS
DOCUMENT NUMBER: 49:16062
ORIGINAL REFERENCE NO.: 49:3200c-h
TITLE: The structural specificity of vitamin B1. VIII
AUTHOR(S): Dornow, Alfred; Hargesheimer, Alfred
CORPORATE SOURCE: Tech. Hochschule, Hannover, Germany
SOURCE: Chemische Berichte (1953), 86, 461-5
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C.A. 44, 2530b. Three vitamin B1 analogs and 3 B1 antagonists are

described. HOCH:CHAc condensed with EtO2CCH2C(:NH)OEt (I) gave 32% Et 2-amino-6-methylnicotinate (II), m. 88° (cf. C.A. 34, 6629.2). II (2.2 g.) and 0.6 g. LiAlH4 in Et2O yielded 1.4 g. 6-methyl-3-hydroxymethyl-2-aminopyridine (III), m. 98°; HCl salt, m. 170.5°. III (0.5 g.) in Et2O refluxed with 5 cc. SOCl2 gave 0.45 g. 6-methyl-3-chloromethyl-2-aminopyridine-HCl (IV), m. 162°. IV (0.2 g.) and 0.15 g. 4-methyl-5-(β-hydroxyethyl)thiazole(V) in 20 cc. MeNO2 12 hrs. at 40° gave 0.26 g. of the vitamin B1 analog, 4-methyl-5-(β-hydroxyethyl)-3-(2-amino-6-methyl-3-pyridylmethyl)thiazolium chloride-HCl, m. 225°, which had 1/5000 the activity of vitamin B1 in the Lactobacillus fermenti test. Similarly, 2 g. Et 6-phenyl-2-aminonicotinate (31% from I and BzCH2CHO) with 0.93 g. LiAlH4 yielded 1.5 g. 3-hydroxymethyl-6-phenyl-2-aminopyridine (VI), m. 76°; HCl salt, m. 300° (decomposition). VI (0.9 g.) and 0.53 g. SOCl2 refluxed in Et2O gave 0.8 g. 3-chloro-methyl-6-phenyl-2-aminopyridine-HCl (VII), m. 284° (decomposition). VII (0.2 g.) and 0.12 g. of V in iso-PrOH at 50-60° several min. gave 0.27 g. 4-methyl-5-(β-hydroxyethyl)-3-(2-amino-6-phenyl-3-pyridylmethyl)thiazolium chloride-HCl, m. 213°, having 1/16000 the activity of vitamin B1. The 4,6-dimethyl analog of III [m. 120°; picrate, m. 175°; HCl salt, m. 188° (decomposition); HBr salt, m. 222°] when refluxed in 50 cc. CHCl3 with 10 cc. SOCl2 gave 88% 4,6-dimethyl-3-chloromethyl-2-aminopyridine-HCl (VIII), m. 196°. VIII (0.15 g.) and 0.2 g. V in MeNO2 17 hrs. at room temperature gave 0.16 g. 4-methyl-5-(β-hydroxyethyl)-3-[2-amino-4,6-dimethyl-3-pyridylmethyl)thiazolium chloride-HCl, m. 214°, having 1/47000 the activity of vitamin B1. To prepare vitamin B1 antagonists, IV, VII, and VIII were each heated with 2-methyl-3-(β-hydroxyethyl)pyridine in MeNO2 to give, resp., 24% 2-methyl-2-(β-hydroxyethyl)-1-(2-amino-6-methyl-3-pyridylmethyl)pyridinium chloride-HCl, m. 196°, having 1/300 the activity of the antivitamin B1, neopyrithiamine (cf. C.A. 44, 2530b, 4472e); 43% 1-(2-amino-6-phenyl-3-pyridylmethyl) analog, m. 262° (decomposition); and 42% 1-(2-amino-4,6-dimethyl-3-pyridylmethyl) analog, m. 202°, having 1/370 the activity of neopyrithiamine.

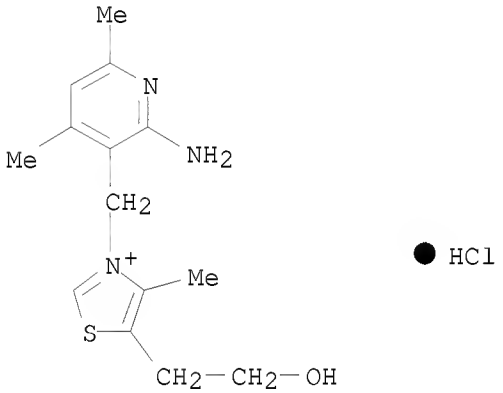
IT 13860-66-7P, Thiazolium, 3-[(2-amino-6-methyl-3-pyridyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride 109402-01-9P, Thiazolium, 3-[(2-amino-4,6-dimethyl-3-pyridyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride
RL: PREP (Preparation)
(preparation of)

RN 13860-66-7 CAPLUS

CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



RN 109402-01-9 CAPLUS
CN Thiazolium, 3-[(2-amino-4,6-dimethyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

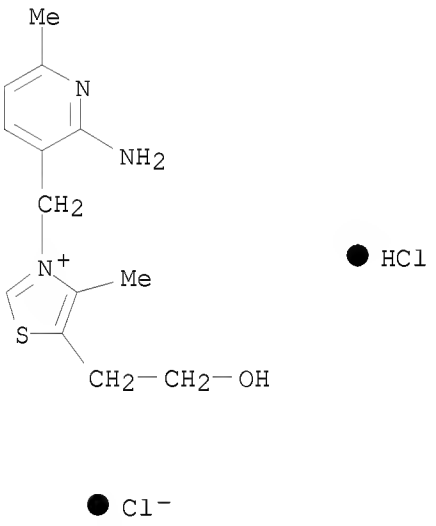
L7 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1951:27026 CAPLUS
DOCUMENT NUMBER: 45:27026
ORIGINAL REFERENCE NO.: 45:4724f-i
TITLE: Syntheses of vitamin B1 and its related compounds. III. Synthesis of a new heterovitamin B1
AUTHOR(S): Matsukawa, Taizo; Matsuno, Toshimasa
CORPORATE SOURCE: Research Lab., Ch. Takeda & Co., Osaka
SOURCE: Yakugaku Zasshi (1944), 64, 145-51
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Condensation of the Na salt of MeCOCH2CHO and NCCH2CN gives

2-methyl-5-cyano-6-hydroxypyridine, decompose 292-3°, which, with POCl3 yields the 6-Cl compound (I), m. 114-15°. I with alc. NH3 gives the 6-amino compound (II), m. 185.5-6°. Electrolytic reduction of II in HCl solution with Pd black as the anode, as described in Part I (cf. preceding abstract), yields 2-methyl-5-aminomethyl-6-aminopyridine-2HCl (III), decompose 273-3.5°; dipicrate, decompose 215-16°. III with H3PO4 and NaO2CH gives 2-methyl-5-formamidomethyl-6-aminopyridine (IV), m. 165-5.5°; dipicrate decompose 214°. III in water with KHCO3 and HCSSK III gives 2-methyl-5-thioformamidomethyl-6-aminopyridine (V), decompose 130°. II treated with AcCH(SH)CH2CH2OAc or 2-methyl-2-hydroxy-3-acetyl-3-mercaptotetrahydrofuran and then with HCl gives 4-methyl-5-(2-hydroxyethyl)-3-[(2-methyl-6-amino-5-pyridyl)methyl]thiazolium chloride-HCl (VI), decompose 225°. VI gives a strongly pos. formaldehyde-azo test and properties similar to those of vitamin B1. It can also be obtained by the condensation of V and AcCHClCH2CH2CH2OAc or 2-methyl-2-hydroxy-3-acetyl-3-chlorotetrahydrofuran.

IT 13860-66-7P, Thiazolium, 3-[(2-amino-6-methyl-3-pyridyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride
RL: PREP (Preparation)
(preparation of)

RN 13860-66-7 CAPLUS

CN Thiazolium, 3-[(2-amino-6-methyl-3-pyridinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-, chloride, hydrochloride (1:1:1) (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

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---Logging off of STN---

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Executing the logoff script...

=> LOG Y

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	154.46	393.19

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-13.60	-13.60

STN INTERNATIONAL LOGOFF AT 16:27:12 ON 21 APR 2010